

Full wwPDB X-ray Structure Validation Report (i)

Nov 22, 2021 – 09:03 am GMT

PDB ID : 70YF

Title : Crystal structure of depupylase Dop in complex with Pup and ADP/trifluoro

magnesate

Authors : Cui, H. Deposited on : 2021-06-24

Resolution : 1.88 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org
A user guide is available at

https://www.wwpdb.org/validation/2017/XrayValidationReportHelp with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

MolProbity: 4.02b-467

Mogul : 1.8.4 (270009), CSD as541be (2020)

 $Xtriage\ (Phenix) \quad : \quad 1.13$

EDS : 2.23.2

 $buster-report \quad : \quad 1.1.7 \ (2018)$

Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)

Refmac: 5.8.0267

CCP4 : 7.1.010 (Gargrove)

Ideal geometry (proteins) : Engh & Huber (2001) Ideal geometry (DNA, RNA) : Parkinson et al. (1996)

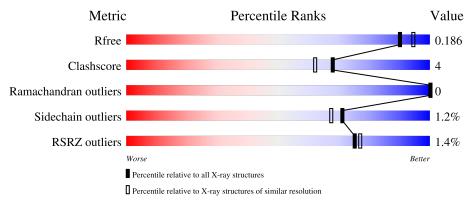
Validation Pipeline (wwPDB-VP) : 2.23.2

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: X- $RAY\ DIFFRACTION$

The reported resolution of this entry is 1.88 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	$\begin{array}{c} \text{Whole archive} \\ (\#\text{Entries}) \end{array}$	Similar resolution $(\# \text{Entries, resolution range}(\text{\AA}))$
R_{free}	130704	9470 (1.90-1.86)
Clashscore	141614	10282 (1.90-1.86)
Ramachandran outliers	138981	10152 (1.90-1.86)
Sidechain outliers	138945	10152 (1.90-1.86)
RSRZ outliers	127900	9303 (1.90-1.86)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain				
1	A	508	84%	% 7%			
2	В	28	89%	11%			



2 Entry composition (i)

There are 10 unique types of molecules in this entry. The entry contains 4462 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

• Molecule 1 is a protein called Depupylase.

Mol	Chain	Residues		Atoms			ZeroOcc	AltConf	Trace	
1	٨	473	Total	С	N	О	S	0	11	0
1	A	413	3822	2395	699	710	18	0	11	0

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	503	GLU	-	expression tag	UNP A0LU48
A	504	ASN	-	expression tag	UNP A0LU48
A	505	LEU	-	expression tag	UNP A0LU48
A	506	TYR	-	expression tag	UNP A0LU48
A	507	PHE	-	expression tag	UNP A0LU48
A	508	GLN	-	expression tag	UNP A0LU48

• Molecule 2 is a protein called Prokaryotic ubiquitin-like protein Pup.

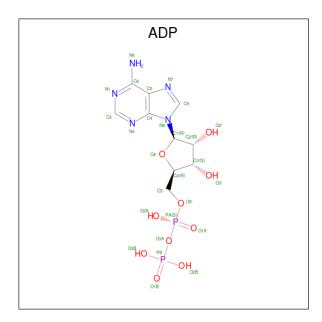
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	Trace		
2	В	28	Total 228	C 140	N 34	O 54	0	1	0

• Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	${f Atoms}$	ZeroOcc	AltConf
3	A	3	Total Mg 3 3	0	0

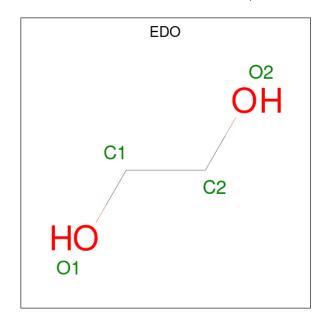
• Molecule 4 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$) (labeled as "Ligand of Interest" by depositor).





Mol	Chain	Residues		Ato	oms			ZeroOcc	AltConf
4	A	1	Total 27	C 10	N 5	O 10	P 2	0	0

 \bullet Molecule 5 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $\mathrm{C_2H_6O_2}).$



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O 4 2 2	0	0
5	A	1	Total C O 4 2 2	0	0
5	A	1	Total C O 4 2 2	0	0

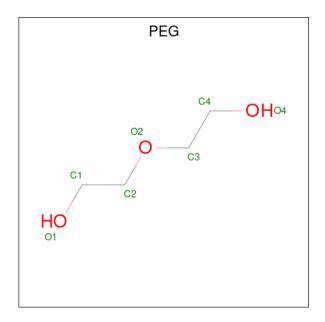
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O 4 2 2	0	0
5	A	1	Total C O 4 2 2	0	0
5	A	1	Total C O 4 2 2	0	0
5	В	1	Total C O 4 2 2	0	0

• Molecule 6 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C O 7 4 3	0	0
6	A	1	Total C O 7 4 3	0	0

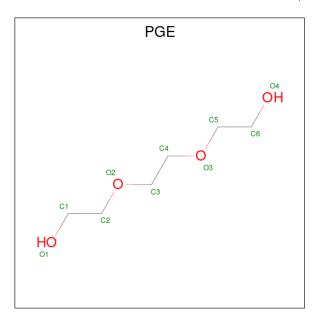
 \bullet Molecule 7 is ACETATE ION (three-letter code: ACT) (formula: $\mathrm{C_2H_3O_2}).$





Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total 4	C 2	O 2	0	0

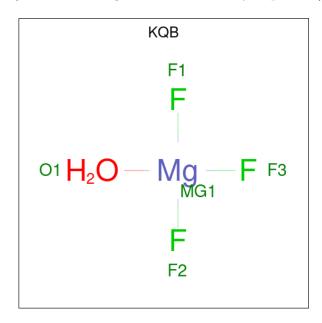
 \bullet Molecule 8 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula: $\mathrm{C_6H_{14}O_4}).$



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	1	Total C O 10 6 4	0	0
8	A	1	Total C O 10 6 4	0	0
8	A	1	Total C O 10 6 4	0	0



• Molecule 9 is trifluoromagnesate monohydrate (three-letter code: KQB) (formula: F₃MgO) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf		
0	Λ	1	Total	F	Mg	О	0	0
9	А	1	5	3	1	1	U	0

• Molecule 10 is water.

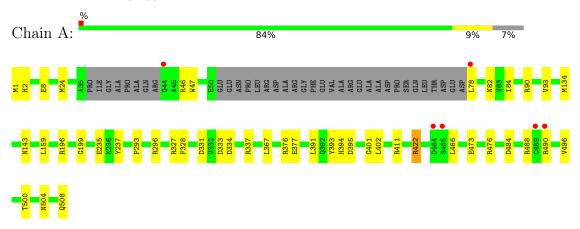
\mathbf{Mol}	Chain	Residues	Atoms	ZeroOcc	AltConf
10	A	278	Total O 278 278	0	0
10	В	23	Total O 23 23	0	0



3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Depupylase



• Molecule 2: Prokaryotic ubiquitin-like protein Pup







4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants	106.33Å 106.33Å 107.38Å	Depositor
a, b, c, α , β , γ	90.00° 90.00° 120.00°	Depositor
Resolution (Å)	47.65 - 1.88	Depositor
Resolution (A)	47.65 - 1.88	EDS
% Data completeness	100.0 (47.65-1.88)	Depositor
(in resolution range)	100.0 (47.65-1.88)	EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	2.15 (at 1.88Å)	Xtriage
Refinement program	PHENIX 1.19_4092	Depositor
D.D.	0.159 , 0.188	Depositor
R, R_{free}	0.158 , 0.186	DCC
R_{free} test set	2960 reflections (5.15%)	wwPDB-VP
Wilson B-factor (Å ²)	29.5	Xtriage
Anisotropy	0.254	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$, $B_{sol}(Å^2)$	(Not available), (Not available)	EDS
L-test for twinning ²	$< L >=0.50, < L^2>=0.33$	Xtriage
Estimated twinning fraction	0.022 for -h,-k,l	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	4462	wwPDB-VP
Average B, all atoms (Å ²)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 4.35% of the height of the origin peak. No significant pseudotranslation is detected.

²Theoretical values of <|L|>, $<L^2>$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.



¹Intensities estimated from amplitudes.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: ACT, MG, KQB, EDO, PGE, ADP, PEG

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with |Z| > 5 is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mal	Chain	Bo	nd lengths	Bond angles		
Mol Chain		RMSZ	# Z > 5	RMSZ	# Z > 5	
1	A	0.49	1/3934 (0.0%)	0.71	1/5333 (0.0%)	
2	В	0.52	0/232	0.66	0/310	
All	All	0.49	1/4166 (0.0%)	0.71	1/5643 (0.0%)	

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$\operatorname{Observed}(\text{\AA})$	$Ideal(\AA)$
1	A	8	GLU	CD-OE2	-6.79	1.18	1.25

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^o)$	$\operatorname{Ideal}({}^{o})$
1	A	8	GLU	OE1-CD-OE2	-6.16	115.91	123.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3822	0	3767	29	1
2	В	228	0	208	4	0
3	A	3	0	0	0	0
4	A	27	0	12	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	24	0	36	0	0
5	В	4	0	6	0	0
6	A	14	0	20	0	0
7	A	4	0	3	0	0
8	A	30	0	42	4	0
9	A	5	0	0	0	0
10	A	278	0	0	3	0
10	В	23	0	0	0	0
All	All	4462	0	4094	31	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

All (31) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:82:ASN:HD21	1:A:90:ARG:HH21	1.07	0.97
1:A:422:ARG:NH1	10:A:701:HOH:O	2.04	0.85
1:A:391[B]:LEU:HD23	2:B:61:PHE:HE1	1.62	0.64
1:A:473[A]:GLU:HG2	1:A:476:ARG:HG3	1.84	0.60
1:A:391[B]:LEU:HD23	2:B:61:PHE:CE1	2.36	0.60
1:A:47:TRP:CE3	1:A:84:ILE:HD11	2.39	0.58
1:A:393:TYR:HA	1:A:402:LEU:HB2	1.89	0.55
1:A:504:ASN:HA	1:A:508:GLN:HG2	1.88	0.55
1:A:466:LEU:O	8:A:615:PGE:H3	2.06	0.55
1:A:159:LEU:HD13	4:A:604:ADP:HN62	1.74	0.52
1:A:496:VAL:O	1:A:500:THR:HG23	2.12	0.50
1:A:78:LEU:N	10:A:711:HOH:O	2.45	0.50
1:A:376[B]:ARG:NH2	1:A:377:GLU:OE2	2.37	0.49
1:A:24:MET:CE	1:A:93:VAL:HG11	2.43	0.48
1:A:367:LEU:HD21	8:A:614:PGE:H1	1.95	0.48
2:B:68:LYS:HA	2:B:68:LYS:HE2	1.95	0.47
1:A:334:ASP:OD1	1:A:337:ARG:NH1	2.47	0.47
1:A:484:ASP:O	1:A:488:ARG:HG3	2.14	0.46
1:A:395:ASP:HB3	1:A:401:GLY:HA2	1.98	0.45
1:A:328:PHE:O	1:A:331:ASP:HB3	2.17	0.44
1:A:2:HIS:ND1	10:A:704:HOH:O	2.36	0.44
1:A:296:ARG:HE	1:A:296:ARG:HB2	1.59	0.44
1:A:159:LEU:HD11	1:A:237:TYR:HB3	2.00	0.43
1:A:199:GLY:HA3	8:A:614:PGE:H52	2.01	0.43
1:A:1:MET:N	1:A:333:ASP:OD2	2.47	0.42

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Continued	trom	mmoninonic	maaa
COHABABACA		DIEUIUU	DUIUE
0 0 1000100000			

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:46:ILE:HD12	2:B:46:ILE:HA	1.83	0.41
1:A:490:ARG:HE	1:A:490:ARG:HB2	1.72	0.41
1:A:24:MET:HE1	1:A:93:VAL:HG11	2.02	0.41
1:A:293:PRO:HG2	8:A:614:PGE:H32	2.03	0.41
1:A:143:ASN:HB3	1:A:394:HIS:CG	2.56	0.41
1:A:47:TRP:CZ3	1:A:84:ILE:HD11	2.56	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	$\begin{array}{c} \text{Clash} \\ \text{overlap } (\text{\AA}) \end{array}$
1:A:235:GLU:OE1	1:A:327:ARG:NH2[5_674]	2.00	0.20

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Perce	ntiles
1	A	478/508 (94%)	471 (98%)	7 (2%)	0	100	100
2	В	27/28 (96%)	27 (100%)	0	0	100	100
All	All	505/536~(94%)	498 (99%)	7 (1%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.



Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	$404/420 \ (96\%)$	399 (99%)	5 (1%)	71	67
2	В	25/24 (104%)	25 (100%)	0	100	100
All	All	429/444 (97%)	424 (99%)	5 (1%)	71	67

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	46	ARG
1	A	134	MET
1	A	196	ARG
1	A	411	ARG
1	A	422	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	2	HIS
1	A	82	ASN
1	A	375	GLN
1	A	426	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 18 ligands modelled in this entry, 3 are monoatomic - leaving 15 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.



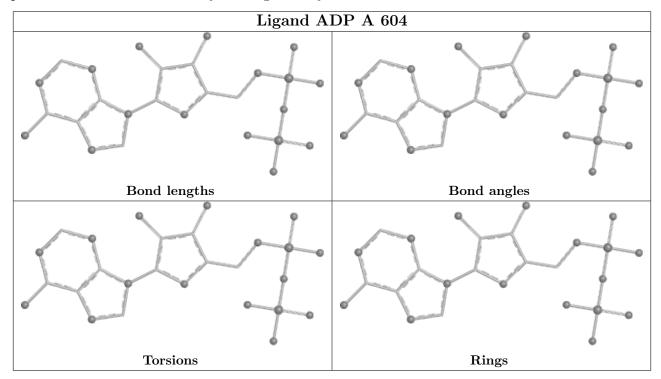
There are no chirality outliers.

There are no torsion outliers.

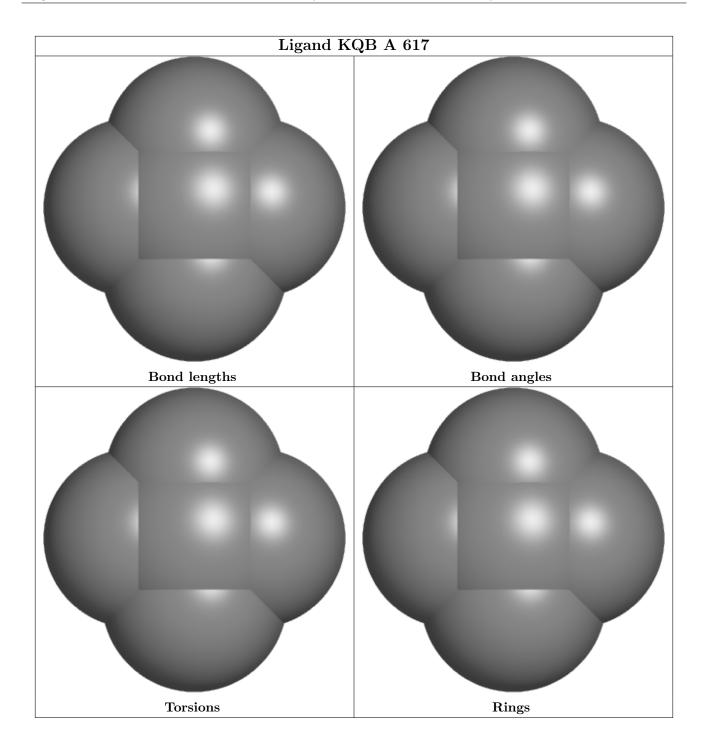
There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.







5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.



6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled '#RSRZ>2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	$\langle { m RSRZ} \rangle$	$\# \mathrm{RSRZ}{>}2$	$OWAB(A^2)$	Q<0.9
1	A	473/508 (93%)	-0.23	6 (1%) 77 79	21, 29, 52, 84	6 (1%)
2	В	28/28 (100%)	-0.18	1 (3%) 42 44	24, 33, 51, 70	0
All	All	501/536 (93%)	-0.23	7 (1%) 75 77	21, 29, 52, 84	6 (1%)

All (7) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	В	44	ASP	4.3
1	A	78	LEU	3.4
1	A	464	ASP	3.4
1	A	490	ARG	2.8
1	A	44	GLN	2.4
1	A	489	CYS	2.2
1	A	465	SER	2.2

6.2 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.



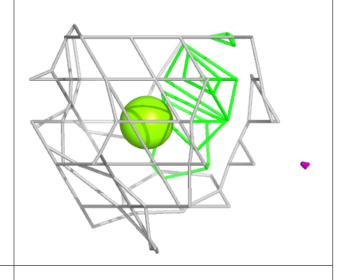
Mol	Type	Chain	Res	Atoms	RSCC	RSR	$\mathbf{B} ext{-}\mathbf{factors}(\mathring{\mathbf{A}}^2)$	Q < 0.9
5	EDO	A	609	4/4	0.58	0.31	63,65,69,69	0
5	EDO	A	610	4/4	0.66	0.38	47,50,56,57	0
7	ACT	A	613	4/4	0.67	0.21	60,65,74,74	0
5	EDO	В	101	4/4	0.69	0.26	59,60,60,63	0
5	EDO	A	606	4/4	0.69	0.39	59,61,61,68	0
8	PGE	A	615	10/10	0.78	0.18	65,67,73,76	0
5	EDO	A	605	4/4	0.80	0.20	52,55,56,58	0
5	EDO	A	607	4/4	0.83	0.18	48,55,57,62	0
6	PEG	A	612	7/7	0.83	0.15	52,58,67,68	0
8	PGE	A	616	10/10	0.84	0.16	60,65,69,73	0
6	PEG	A	611	7/7	0.86	0.20	46,49,53,65	0
8	PGE	A	614	10/10	0.88	0.45	46,54,58,58	0
3	MG	A	603	1/1	0.89	0.15	23,23,23,23	1
5	EDO	A	608	4/4	0.93	0.18	34,36,43,50	0
3	MG	A	601	1/1	0.94	0.05	25,25,25,25	0
3	MG	A	602	1/1	0.96	0.06	26,26,26,26	0
9	KQB	A	617	5/5	0.96	0.07	27,29,31,36	0
4	ADP	A	604	27/27	0.98	0.06	24,28,35,36	0

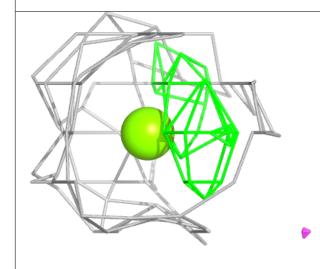
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

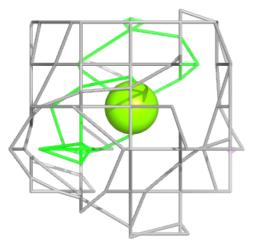


Electron density around MG A 603: $2 \mathrm{mF}_o\text{-DF}_c \text{ (at } 0.7 \mathrm{\ rmsd) in gray}$ $\mathrm{mF}_o\text{-DF}_c \text{ (at } 3 \mathrm{\ rmsd) in purple (negative)}$

and green (positive)



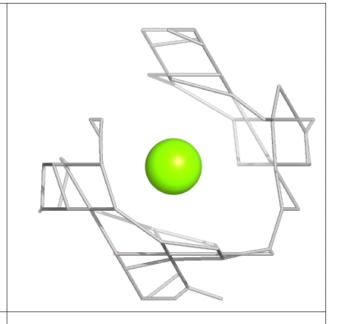


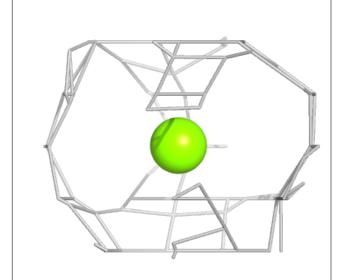


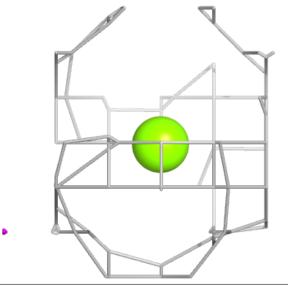


Electron density around MG A 601:

 $2 {
m mF}_o {
m -DF}_c$ (at 0.7 rmsd) in gray ${
m mF}_o {
m -DF}_c$ (at 3 rmsd) in purple (negative) and green (positive)



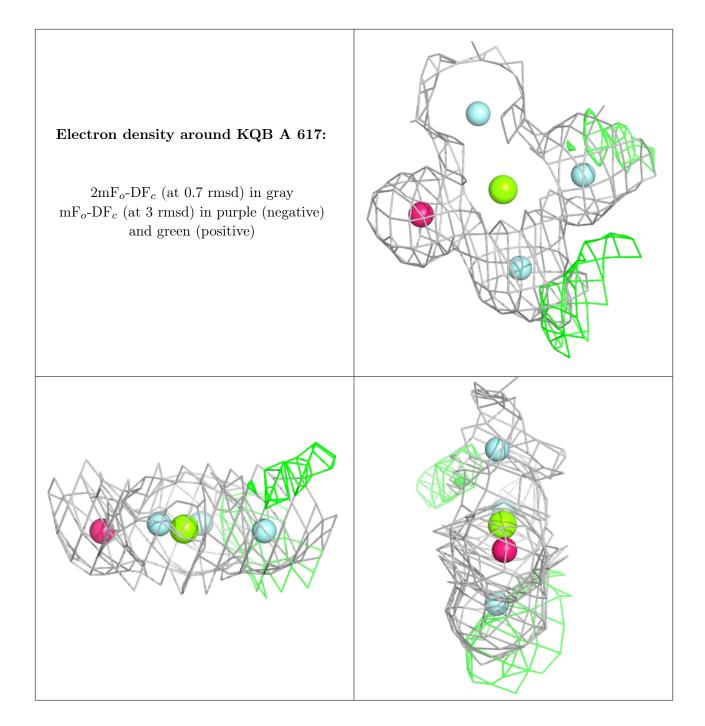




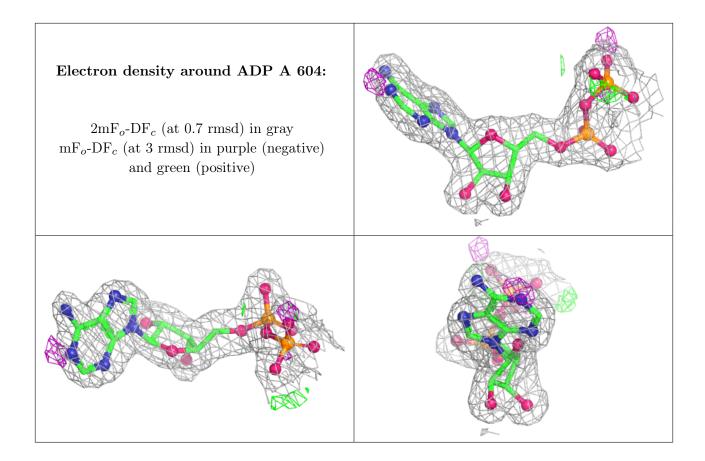


Electron density around MG A 602: 2mF_o-DF_c (at 0.7 rmsd) in gray mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)









6.5 Other polymers (i)

There are no such residues in this entry.

